Supporting Information

Structural Evolution, Sequential Oxidation and Chemical Bonding in Tri-yttrium Oxide Clusters: $Y_3O_x^-$ and Y_3O_x ($x = 0-6$)

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Figure S1-S7 Isomeric structures and their relative energies 0.40 eV above the ground state for $Y_3O_x^{-/0}$ ($x = 0$-6).

Figure S8 The simulated photoelectron spectra for $Y_3O_x^-$ ($x = 0$-5) selected low-lying structures except for the ground state (within ~0.10 eV). The simulations are done by fitting the distribution of calculated vertical detachment energies with unit-area Gaussian functions of 0.10 eV width.

Table SI Relative energies of the low-lying states of the $Y_3O_x^{/0}$ ($x = 0-2$) clusters at the BP86 level (within 0.20 eV), and comparisons with those from the CCSD(T) single-point calculations(with 0.20 eV) at the BP86 geometries.

Table SII Cartesian coordinates for the all optimized structures within 0.40 eV for $Y_3O_x^{-/0}$ ($x = 0-5$) at the BP86/Y/Stuttgart+2f1g/O/aug-cc-pvTZ level of theory.
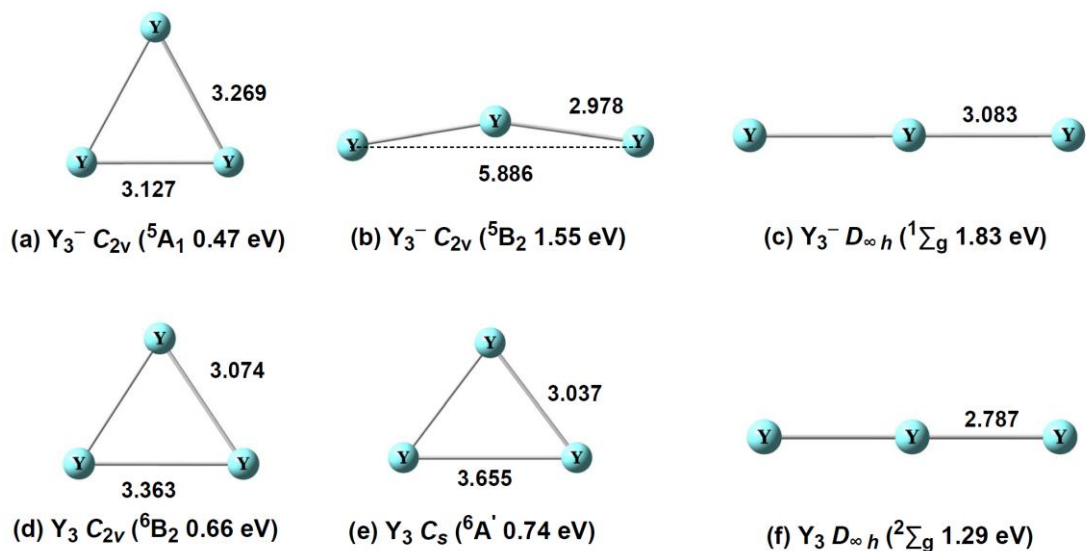
Figure S1 Isomeric structures and their relative energies for $Y_3^{-/0}$.

Figure S2 Isomeric structures and their relative energies for $Y_3O^{-/0}$.

(a) $Y_3O_2^-$ C_s ($^5A'$ 0.41 eV)   (b) $Y_3O_2^-$ C_s ($^3A'$ 1.88 eV)   (c) $Y_3O_2^-$ C_s ($^1A'$ 2.01 eV)   (d) Y_3O_2 C_s ($^2A'$ 0.43 eV)

(e) Y_3O_2 C_{2v} ($^4B_2$ 0.65 eV)   (f) Y_3O_2 C_{2v} ($^4A_1$ 1.04 eV)   (g) Y_3O_2 C_s ($^6A'$ 1.04 eV)   (h) Y_3O_2 C_s ($^6A''$ 1.06 eV)

(i) Y_3O_2 C_{2v} ($^6A_2$ 1.07 eV)   (j) Y_3O_2 C_{2v} ($^4B_2$ 1.22 eV)

Figure S3 Isomeric structures and their relative energies for $Y_3O_2^{-/0}$.

(a) $Y_3O_3^- C_s$ ($^1A'$ 0.86 eV)

(b) $Y_3O_3^- C_s$ ($^5A''$ 0.86 eV)

(c) $Y_3O_3^- C_{2v}$ ($^1A_1$ 1.04 eV)

(d) $Y_3O_3^- C_s$ ($^3A'$ 1.05 eV)

(e) $Y_3O_3^- C_s$ ($^5A''$ 1.54 eV)

(f) $Y_3O_3^- C_s$ ($^1A'$ 1.74 eV)

(g) $Y_3O_3^- C_s$ ($^1A'$ 1.89 eV)

(h) $Y_3O_3 C_s$ ($^4A''$ 0.45 eV)

(i) $Y_3O_3 C_s$ ($^2A'$ 0.56 eV)

(j) $Y_3O_3 C_{2v}$ ($^2B_2$ 0.59 eV)

(k) $Y_3O_3 C_{2v}$ ($^4B_2$ 1.28 eV)

(l) $Y_3O_3 C_s$ ($^4A'$ 1.61 eV)

Figure S4 Isomeric structures and their relative energies for $Y_3O_3^{-/0}$.

(a) $Y_3O_4^- C_1$ (^3A 2.19 eV)

(b) $Y_3O_4^- C_s$ ($^1A'$ 2.20 eV)

(c) $Y_3O_4^- C_s$ ($^1A'$ 2.25 eV)

(d) $Y_3O_4^- C_s$ ($^1A'$ 3.93 eV)

(e) $Y_3O_4 C_{2v}$ ($^2A_1$ 0.52 eV)

(f) $Y_3O_4 D_{2d}$ ($^2A_1$ 1.52 eV)
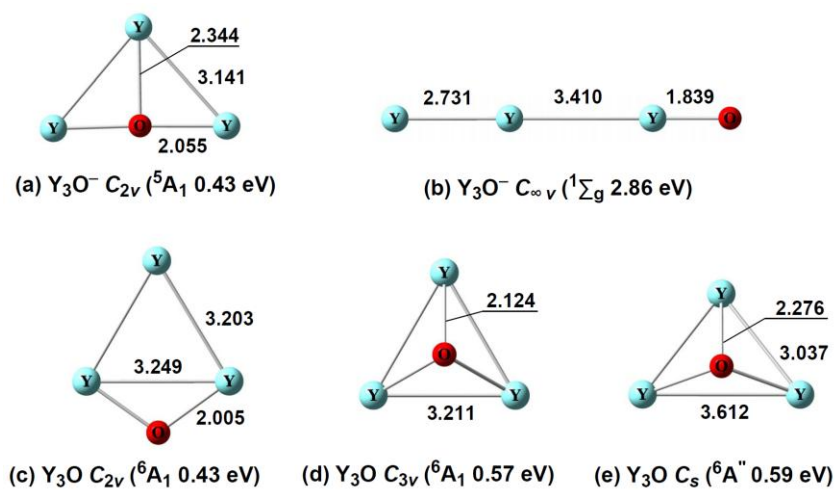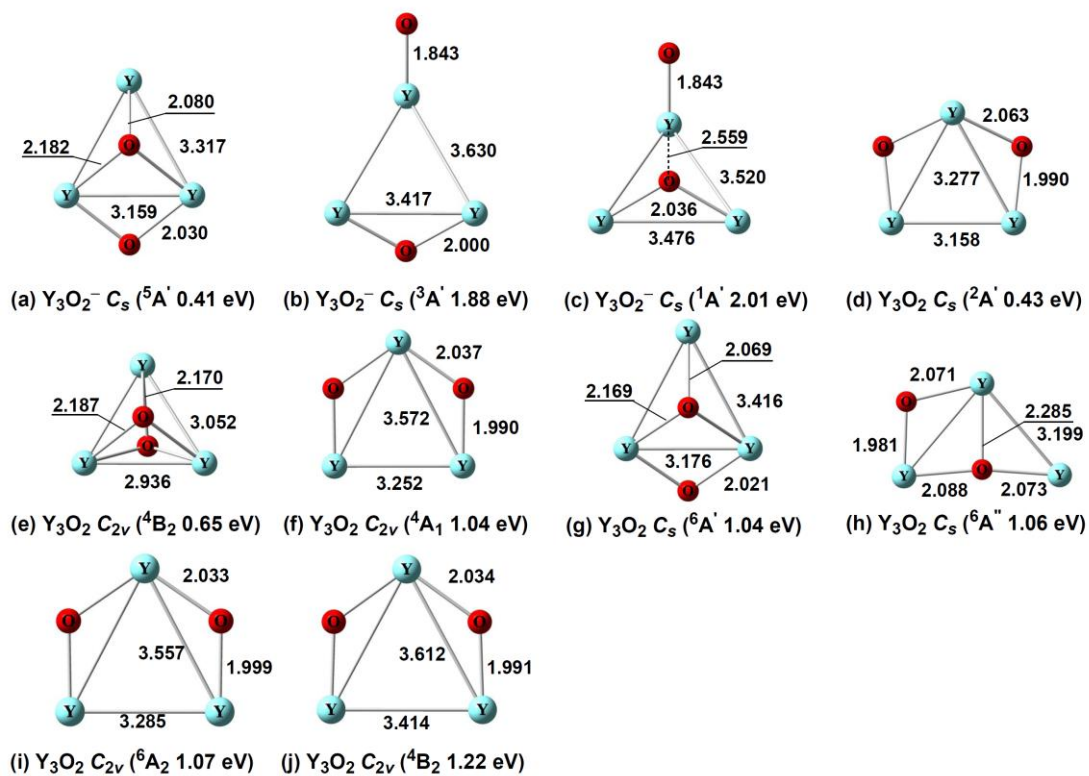
(g) $Y_3O_4 C_{2v}$ ($^4B_1$ 3.47 eV)

Figure S5 Isomeric structures and their relative energies for $Y_3O_4^{-/0}$.

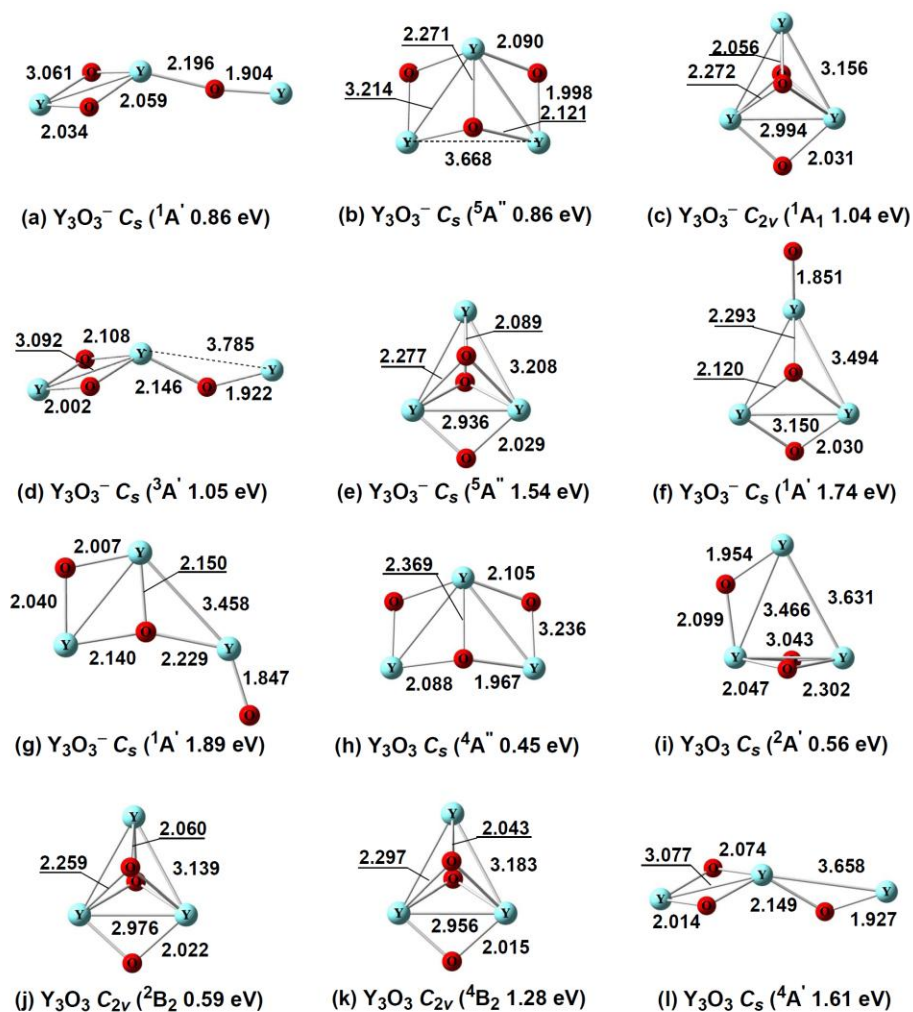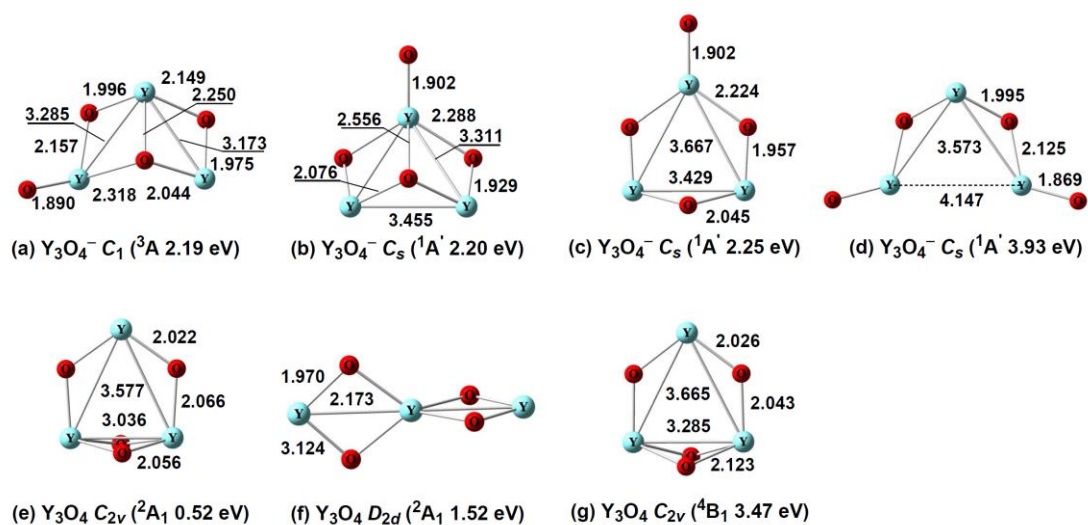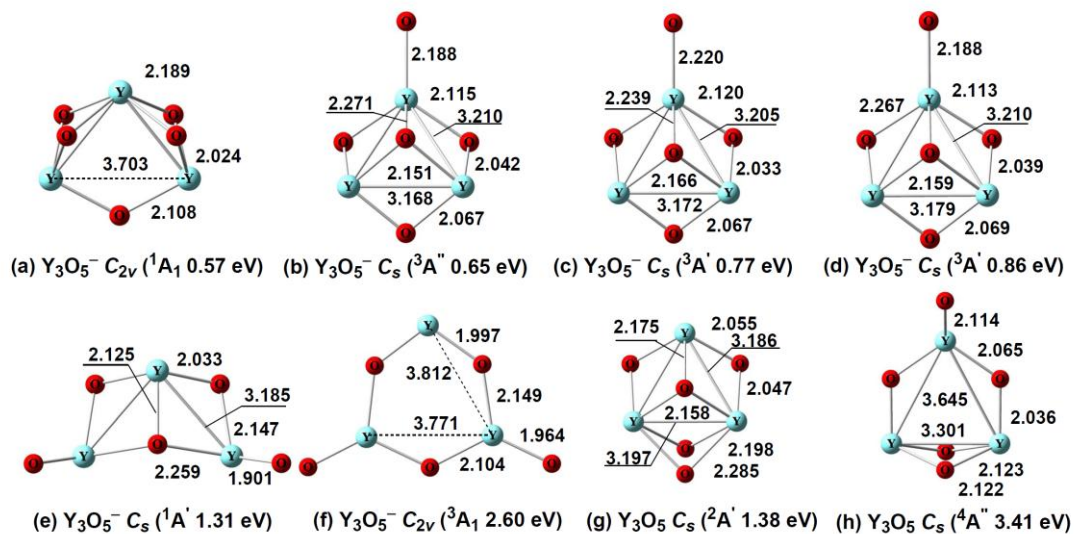**Figure S6** Isomeric structures and their relative energies for $Y_3O_5^{-/0}$.

(a) $Y_3O_5^-$ C_{2v} ($^1A_1$ 0.57 eV) (b) $Y_3O_5^-$ C_s ($^3A''$ 0.65 eV) (c) $Y_3O_5^-$ C_s ($^3A'$ 0.77 eV) (d) $Y_3O_5^-$ C_s ($^3A'$ 0.86 eV)

(e) $Y_3O_5^-$ C_s ($^1A'$ 1.31 eV) (f) $Y_3O_5^-$ C_{2v} ($^3A_1$ 2.60 eV) (g) Y_3O_5 C_s ($^2A'$ 1.38 eV) (h) Y_3O_5 C_s ($^4A''$ 3.41 eV)

Figure S7 Isomeric structures and their relative energies for $Y_3O_6^{-/0}$.

(a) $Y_3O_6^-$ C_s ($^3A'$ 0.48 eV) (b) $Y_3O_6^-$ C_{2v} ($^1A_1$ 0.54 eV) (c) $Y_3O_6^-$ C_1 (^1A 0.65 eV) (d) Y_3O_6 C_s ($^2A''$ 1.47 eV)

(e) $Y_3O_6^-$ C_s ($^3A''$ 0.77 eV) (f) Y_3O_6 C_s ($^2A'$ 0.72 eV) (g) Y_3O_6 C_s ($^2A''$ 1.47 eV)

Figure S8

(a) Y_3O^-
C_{2v} ($^3B_1$ 0.05 eV)

(b) $Y_3O_2^-$
C_s ($^1A'$ 0.07 eV)

(c) $Y_3O_2^-$
C_s ($^1A'$ 0.02 eV)

(d) $Y_3O_3^-$
C_{3v} ($^3A''$ 0.02 eV)

(e) $Y_3O_4^-$
C_s (3A'' 0.00 eV)

(f) $Y_3O_4^-$
C_s ($^3A'$ 0.06 eV)

Binding Energy (eV)

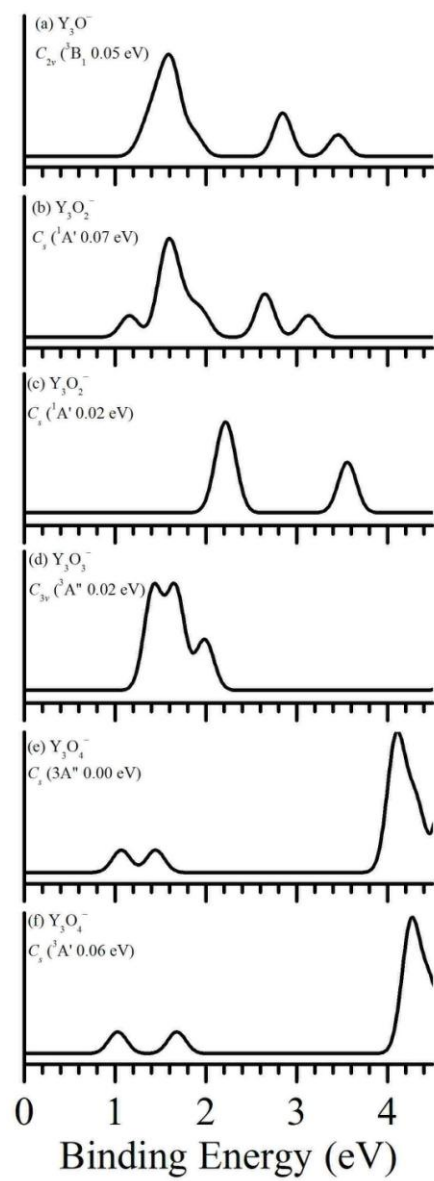**Table SI** Relative energies of the low-lying states of the $Y_3O_x^{-/0}$ ($x = 0$–2) clusters at the BP86 level (within 0.20 eV), and comparisons with those from the CCSD(T) single-point calculations(with ~ 0.20 eV) at the BP86 geometries.

Cluster	Symmetry	State	BP86 [a,b]	CCSD(T) [a,c]
Y_3	D_{3h}	$^2A_1'$	0.00	0.00
	D_{3h}	$^2A_2''$	0.10	0.08
	C_{3v}	$^1A_1$	0.00	0.00 (0.00)[d]
Y_3O^-	C_{2v}	$^3B_1$	0.05	0.00 (0.02)[d]
	C_s	$^3A''$	0.07	0.10 (0.10)[d]
	C_s	$^1A'$	0.00	0.00
$Y_3O_2^-$	C_s	$^1A'$	0.02	0.24
	C_s	$^3A''$	0.18	0.55
	C_s	$^3A'$	0.20	0.57
	C_s	$^2A'$	0.00	0.00
Y_3O_2	C_{2v}	$^4A_2$	0.06	0.31
	C_s	$^4A''$	0.16	0.48
$Y_3O_3^-$	C_s	$^3A''$	0.00	0.00
	C_{3v}	$^1A_1$	0.02	0.18
Y_3O_3	C_s	$^2A''$	0.00	0.00
	C_s	$^2A'$	0.04	0.15
	C_{3v}	$^1A_1$	0.00	0.00
$Y_3O_4^-$	C_s	$^3A''$	0.00	0.18
	C_s	$^3A'$	0.06	0.25
Y_3O_5	C_s	$^2A''$	0.00	0.00
	C_s	$^2A'$	0.11	0.31
$Y_3O_6^-$	C_s	$^1A'$	0.00	0.00
	C_s	$^3A''$	0.06	0.60

[a] All energies are in eV.

[b] At theBP86/Y/Stuttgart+$2f1g$/O/aug-cc-pVTZ level.

[c] Single point CCSD(T) energy using BP86 results within 0.20 eV .

[d] CCSD(T) optimization calculations of Y_3O^-

Table S II. Cartesian coordinates for the all optimized structures within 0.40 eV for $Y_3O_x^{-/0}$ ($x = 0$–5) at the BP86/Y/Stuttgart+$2f1g$/O/aug-cc-pvTZ level of theory.

Cartesian coordinates (Å) of alternative $Y_3O_x^{-/0}$ structures

	x	y	z		x	y	z
Y_3^- D_{3h} ($^1A_1'$ 0.00 eV)				**Y_3 D_{3h} ($^2A_2''$ 0.10 eV)**			
Y	0.000000	1.786178	0.000000	Y	0.000000	1.833747	0.000000
Y	1.546876	-0.893089	0.000000	Y	-1.588072	-0.916874	0.000000
Y	-1.546876	-0.893089	0.000000	Y	1.588072	-0.916874	0.000000
Y_3^- D_{3h} ($^3A_2''$ 0.27 eV)				**Y_3 D_{3h} ($^4A_2''$ 0.27 eV)**			
Y	0.000000	1.822350	0.000000	Y	0.000000	1.609661	-0.929349
Y	1.578201	-0.911175	0.000000	Y	0.000000	0.000000	1.858698
Y	-1.578201	-0.911175	0.000000	Y	0.000000	-1.609661	-0.929349
Y_3^- D_{3h} ($^3A_1'$ 0.34 eV)				**Y_3 C_{2v} ($^4B_2$ 0.31 eV)**			
Y	0.000000	1.817161	0.000000	Y	0.000000	0.000000	1.798438
Y	1.573708	-0.908581	0.000000	Y	0.000000	1.676402	-0.899219
Y	-1.573708	-0.908581	0.000000	Y	0.000000	-1.676402	-0.899219
Y_3^- C_{2v} ($^3A_2$ 0.34 eV)				**Y_3O^- C_{3v} ($^1A_1$ 0.00 eV)**			
Y	0.000000	0.000000	1.781257	Y	0.000000	1.813827	-0.074687
Y	0.000000	1.623013	-0.890629	Y	-1.570820	-0.906913	-0.074687
Y	0.000000	-1.623013	-0.890629	Y	1.570820	-0.906913	-0.074687
				O	0.000000	0.000000	1.092303
Y_3 D_{3h} ($^2A_1'$ 0.00 eV)							
Y	0.000000	1.824507	0.000000				
Y	-1.580070	-0.912254	0.000000	**Y_3O^- C_{2v} ($^3B_1$ 0.05 eV)**			
Y	1.580070	-0.912254	0.000000	Y	0.000000	1.648543	-0.846583
				Y	0.000000	0.000000	2.099996
				Y	0.000000	-1.648543	-0.846583

O   0.000000   0.000000   -1.983300

Y₃O⁻ Cₛ (³A'' 0.07 eV)

Y	0.661710	-0.625445	1.698788
Y	-1.459156	1.120718	0.000000
Y	0.661710	-0.625445	-1.698788
O	0.661710	0.634590	0.000000

Y₃O⁻ C₂ᵥ (¹A₁ 0.22 eV)

Y	0.000000	0.000000	2.067547
Y	0.000000	1.604544	-0.825742
Y	0.000000	-1.604544	-0.825742
O	0.000000	0.000000	-2.028311

Y₃O⁻ Cₛ (³A'' 0.24 eV)

Y	2.024351	0.896397	0.000000
Y	-2.062448	0.739885	0.000000
Y	0.038097	-1.740200	0.000000
O	0.000000	0.506597	0.000000

Y₃O⁻ C₃ᵥ (³A₁ 0.31 eV)

Y	0.000000	2.027291	-0.036423
Y	1.755686	-1.013646	-0.036423
Y	-1.755686	-1.013646	-0.036423
O	0.000000	0.000000	0.532682

Y₃O⁻ Cₛ (⁵A' 0.40 eV)

Y	0.620416	-0.775737	1.551672
Y	0.620416	-0.775737	-1.551672
Y	-1.368096	1.407483	0.000000

O   0.620416   0.701953   0.000000

Y₃O C₃ᵥ (²A₁ 0.00 eV)

Y	0.000000	1.849328	-0.069078
Y	-1.601565	-0.924664	-0.069078
Y	1.601565	-0.924664	-0.069078
O	0.000000	0.000000	1.010261

Y₃O C₂ᵥ (⁴B₁ 0.25 eV)

Y	0.000000	1.676426	-0.819033
Y	0.000000	-1.676426	-0.819033
Y	0.000000	0.000000	2.028467
O	0.000000	0.000000	-1.903203

Y₃O₂⁻ Cₛ (¹A' 0.00 eV)

Y	1.310771	1.803693	0.000000
Y	-0.555567	-0.772985	1.604636
Y	-0.555567	-0.772985	-1.604636
O	-0.417665	0.736276	0.000000
O	-0.555567	-1.992681	0.000000

Y₃O₂⁻ Cₛ (¹A' 0.02 eV)

Y	0.259662	-1.051956	1.901018
Y	-0.625853	1.735842	0.000000
Y	0.259662	-1.051956	-1.901018
O	0.259662	0.897169	1.658909
O	0.259662	0.897169	-1.658909

Y₃O₂⁻ Cₛ (³A'' 0.18 eV)

Y	2.101716	0.192932	0.000000

Y   -1.806281   1.571250   0.000000

Y   -0.587591   -1.539685   0.000000

O   1.424263   -1.711537   0.000000

O   0.000000   0.617114   0.000000

Y₃O₂⁻ Cs (⁵A'' 0.34 eV)

Y_3O_2^- Cs (^{5}A'' 0.34 eV)

Y   -0.360933   1.792091   0.000000

Y   0.149749   -1.081683   1.682866

Y   0.149749   -1.081683   -1.682866

O   0.149749   0.904985   1.798290

O   0.149749   0.904985   -1.798290

Y₃O₂⁻ Cₛ (³A' 0.20 eV)

Y_3O_2^- C_s (^{3}A' 0.20 eV)

Y   2.071275   -0.023580   0.000000

Y   -1.603314   1.831635   0.000000

Y   -0.728121   -1.536256   0.000000

O   1.268281   -1.872231   0.000000

O   0.000000   0.547210   0.000000

Y₃O₂ Cₛ (²A' 0.00 eV)

Y_3O_2 C_s (^{2}A' 0.00 eV)

Y   -1.353520   1.581258   0.000000

Y   0.557037   -0.679316   1.598143

Y   0.557037   -0.679316   -1.598143

O   0.557037   0.816209   0.000000

O   0.610262   -1.901508   0.000000

Y₃O₂ C₂ᵥ (⁴A₂ 0.06 eV)

Y_3O_2 C_{2v} (^{4}A$_2$ 0.06 eV)

Y   0.000000   0.000000   1.994770

Y   0.000000   1.720539   -1.164028

Y   0.000000   -1.720539   -1.164028

O   0.000000   1.657869   0.812384

O   0.000000   -1.657869   0.812384

Y₃O₂⁻ C₂ᵥ (³A₂ 0.21 eV)

Y_3O_2^- C_{2v} (^{3}A$_2$ 0.21 eV)

Y   0.000000   0.000000   1.909343

Y   0.000000   1.706021   -1.127623

Y   0.000000   -1.706021   -1.127623

O   0.000000   1.773127   0.843142

O   0.000000   -1.773127   0.843142

Y₃O₂ Cₛ (⁴A'' 0.16 eV)

Y_3O_2 C_s (^{4}A'' 0.16 eV)

Y   0.538767   -0.685123   1.577992

Y   -1.371205   1.588778   0.000000

Y   0.538767   -0.685123   -1.577992

O   0.892882   -1.885980   0.000000

O   0.538767   0.820638   0.000000

Y₃O₂⁻ C₂ (¹A 0.32 eV)

Y_3O_2^- C_2 (^{1}A 0.32 eV)

Y   0.000000   3.363850   -0.565371

Y   0.000000   0.000000   1.085947

Y   0.000000   -3.363850   -0.565371

O   0.709283   1.695045   0.109186

O   -0.709283   -1.695045   0.109186

O   0.275088   1.145059   1.869708

O   0.275088   1.145059   -1.869708

O   -0.344158   -0.795434   0.000000

Y$_3$O$_2$ C_2 (^{2}A 0.39 eV)

Y   0.000000   3.323519   -0.548276

Y   0.000000   0.000000   1.085004

Y   0.000000   -3.323519   -0.548276

O   0.704516   1.606148   0.028150

O   -0.704516   -1.606148   0.028150

Y$_3$O$_3$ C_s (^{2}A'' 0.00 eV)

Y   0.654949   1.502425   0.000000

Y   -0.339301   -0.906956   1.792618

Y   -0.339301   -0.906956   -1.792618

O   -0.339301   1.096462   1.749817

O   -0.339301   1.096462   -1.749817

O   0.793909   -0.674428   0.000000

Y$_3$O$_3$$^-$ C_s (^{3}A'' 0.00 eV)

Y   -0.670489   1.555409   0.000000

Y   0.347085   -0.924307   1.760216

Y   0.347085   -0.924307   -1.760216

O   0.347085   1.069300   1.756912

O   0.347085   1.069300   -1.756912

O   -0.809620   -0.709221   0.000000

Y$_3$O$_3$$^-$ C_{3v} (^{1}A$_1$ 0.02 eV)

Y   0.000000   2.057113   -0.068388

Y   1.781512   -1.028556   -0.068388

Y   -1.781512   -1.028556   -0.068388

O   1.659708   0.958233   0.333393

O   -1.659708   0.958233   0.333393

O   0.000000   -1.916466   0.333393

Y$_3$O$_3$ C_s (^{2}A' 0.04 eV)

Y   0.007261   -1.078110   1.637314

Y   0.007261   -1.078110   -1.637314

Y   -0.225753   2.121292   0.000000

O   1.015226   -1.710176   0.000000

O   0.007261   0.940224   1.635146

O   0.007261   0.940224   -1.635146

Y$_3$O$_3$$^-$ C_s (^{1}A' 0.32 eV)

Y   -0.592436   1.398985   0.000000

Y   0.275088   -0.852794   2.041935

Y   0.275088   -0.852794   -2.041935

Y$_3$O$_3$ C_s (^{2}A' 0.12 eV)

Y   0.660719   1.604865   0.000000

Y   -0.350451   -0.941552   1.666743

Y   -0.350451   -0.941552   -1.666743

O   -0.350451   1.027043   1.740841

O   -0.350451   1.027043   -1.740841

O   0.896793   -0.697673   0.000000

Y$_3$O$_3$ D_{3h} (^{4}A$_1$' 0.16 eV)

Y   1.861824   1.074924   0.000000

Y   -1.861824   1.074924   0.000000

Y   0.000000   -2.149849   0.000000

O   0.000000   1.868794   0.000000

O   1.618423   -0.934397   0.000000

O   -1.618423   -0.934397   0.000000

Y$_3$O$_4$$^-$ C_{3v} (^{1}A$_1$ 0.00 eV)

Y   0.000000   1.836211   0.071317

Y   1.590206   -0.918106   0.071317

Y   -1.590206   -0.918106   0.071317

O   0.000000   0.000000   1.236168

O   1.672297   0.965501   -0.759728

O   -1.672297   0.965501   -0.759728

O   0.000000   -1.931002   -0.759728

Y$_3$O$_4$$^-$ C_s (^{3}A'' 0.00 eV)

Y   -0.308503   -0.867287   1.599483

Y   -0.308503   -0.867287   -1.599483

Y   0.809550   1.646298   0.000000

O   -1.461127   -1.469510   0.000000

O   -0.308503   1.196568   1.666107

O   -0.308503   1.196568   -1.666107

O   1.139484   -0.493278   0.000000

Y$_3$O$_4$$^-$ C_s (^{3}A' 0.06 eV)

Y   -0.301542   -0.875932   1.581499

Y   -0.301542   -0.875932   -1.581499

Y   0.802439   1.679986   0.000000

O   -1.493390   -1.452438   0.000000

O   -0.301542   1.165409   1.682103

O   -0.301542   1.165409   -1.682103

O   1.124616   -0.527972   0.000000

Y$_3$O$_4$ C_{3v} (^{2}A$_1$ 0.00 eV)

Y   0.000000   1.832621   0.068639

Y   -1.587097   -0.916311   0.068639

Y   1.587097   -0.916311   0.068639

O   -1.664655   0.961089   -0.747240

O   1.664655   0.961089   -0.747240

O   0.000000   -1.922178   -0.747240

O   0.000000   0.000000   1.237876

Y$_3$O$_5$$^-$ C_s (^{1}A' 0.00 eV)

Y   0.700180   1.617271   0.000000

Y   -0.414421   -1.042994   1.567802

Y   -0.414421   -1.042994   -1.567802

O	0.996362	-0.850912	0.000000
O	2.149324	2.886593	0.000000
O	-1.689613	-1.573046	0.000000
O	-0.414421	0.911180	-1.852740
O	-0.414421	0.911180	1.852740

O	-1.253061	-0.206738	0.000000
O	1.677724	-0.682444	0.000000
O	0.242312	-2.462883	0.000000
O	0.229440	1.278202	1.745314
O	0.229440	1.278202	-1.745314

Y_3O_5 C_s ($^2A''$ 0.00 eV)

Y	0.649603	1.553103	0.000000
Y	-0.413401	-1.035704	1.576317
Y	-0.413401	-1.035704	-1.576317
O	0.992287	-0.730349	0.000000
O	2.312744	2.924094	0.000000
O	-1.614386	-1.589437	0.000000
O	-0.413401	0.961215	-1.739572
O	-0.413401	0.961215	1.739572

$Y_3O_6^-$ C_s ($^1A'$ 0.00 eV)

Y	-0.524508	-1.196754	1.564062
Y	-0.524508	-1.196754	-1.564062
Y	0.592573	1.478197	0.000000
O	0.881339	-1.003940	0.000000
O	-1.789194	-1.733125	0.000000
O	-0.524508	0.784069	-1.766059
O	-0.524508	0.784069	1.766059
O	1.594976	3.372676	0.000000
O	2.587058	2.258390	0.000000

Y_3O_5 C_s ($^2A'$ 0.11 eV)

Y	0.686435	1.529567	0.000000
Y	-0.433297	-1.024520	1.579013
Y	-0.433297	-1.024520	-1.579013
O	0.990778	-0.719381	0.000000
O	2.378372	2.908171	0.000000
O	-1.624280	-1.588585	0.000000
O	-0.433297	0.966115	-1.722040
O	-0.433297	0.966115	1.722040

Y_3O_5 C_s ($^2A'$ 0.21 eV)

Y	0.229440	-0.828589	1.505504
Y	0.229440	-0.828589	-1.505504
Y	-0.689824	1.820390	0.000000

$Y_3O_6^-$ C_s ($^3A''$ 0.06 eV)

Y	-0.520641	-1.201445	1.580775

Y	-0.520641	-1.201445	-1.580775
Y	0.547363	1.385650	0.000000
O	0.895462	-0.871111	0.000000
O	-1.732066	-1.757450	0.000000
O	-0.520641	0.832809	-1.729043
O	-0.520641	0.832809	1.729043
O	1.669828	3.446335	0.000000
O	2.615918	2.475650	0.000000

Y$_3$O$_6$$^-$ C_s (^{3}A'' 0.19 eV)

Y	0.780430	1.834095	0.000000
Y	-0.323389	-0.677103	1.626938
Y	-0.323389	-0.677103	-1.626938
O	1.176140	-0.225816	0.000000
O	-0.323389	1.464818	1.666723
O	-1.427671	-1.407292	0.000000
O	-0.323389	1.464818	-1.666723
O	0.123380	-1.817993	3.430130
O	0.123380	-1.817993	-3.430130

Y$_3$O$_6$$^-$ C_s (^{1}A' 0.23 eV)

Y	-0.696686	-1.720996	0.000000
Y	1.709536	-0.005412	0.000000
Y	-1.057647	1.220472	0.000000
O	0.023281	-0.140833	1.338478
O	1.467678	-2.073957	0.000000
O	0.023281	-0.140833	-1.338478
O	-2.411496	-0.470432	0.000000
O	0.023281	3.173110	0.000000
O	1.092362	2.119385	0.000000

Y$_3$O$_6$$^-$ C_s (^{3}A' 0.27 eV)

Y	-0.528871	-1.194508	1.586401
Y	-0.528871	-1.194508	-1.586401
Y	0.553554	1.383383	0.000000
O	0.893566	-0.870955	0.000000
O	-1.729158	-1.763165	0.000000
O	-0.528871	0.837924	-1.720352
O	-0.528871	0.837924	1.720352
O	1.710713	3.423499	0.000000
O	2.640536	2.437237	0.000000

Y$_3$O$_6$ C_s (^{3}A' 0.00 eV)

Y	-0.532736	-1.181299	1.571681
Y	-0.532736	-1.181299	-1.571681
Y	0.539953	1.417378	0.000000
O	0.873411	-0.891259	0.000000
O	-1.738033	-1.739278	0.000000
O	-0.532736	0.816939	-1.719932
O	-0.532736	0.816939	1.719932
O	1.821960	3.329629	0.000000
O	2.670040	2.274980	0.000000